Implementation of the RETRO Anthropogenic Emissions Inventory into the GEOS-Chem Model

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1   Introduction

Anthropogenic VOC emissions in GEOS-Chem are currently derived from a number of global (GEIA, EDGAR) and regional (EPA/NEI, EMEP, STREETS, among others) anthropogenic emissions inventories. Datasets are converted to 2°x2.5° resolution for use in the model, but temporal resolutions vary from monthly to annual between inventories. Aseasonal data (such as in GEIA) are then scaled to simulate monthly resolution. The use of an aseasonal base dataset (GEIA) presents an opportunity for model improvement. Using a base inventory with higher temporal resolution should provide more robust results.

In addition to the lack of monthly resolution, both global datasets employed in the model lack emissions data for a number of NMVOC tracers in the ANTHSRCE diagnostic. As a result, simulated emissions are limited to select geographic regions, usually only the United States and Europe (EPA/NEI and EMEP are the most complete regional datasets).

This document describes the implementation of the RETRO emissions inventory for anthropogenic VOCs into GEOS-Chem. RETRO has monthly temporal resolution and includes a wide suite of speciated VOC emissions, which offer advantages over the global inventories currently employed in the model.

2   Description of RETRO emissions inventory

2.1   Overview

The RETRO (REanalysis of the TROposhperic chemical composition) emissions inventory contains anthropogenic and biomass burning emissions for the years 1960-2000 at 0.5°x0.5° spatial resolution and monthly temporal resolution [1]. For this project, we are concerned with the anthropogenic emissions only. The RETRO team provides all emissions data on their ftp server:

<p style="text-align:center">ftp://ftp.retro.enes.org/pub/emissions/</p>

Emissions are provided in both sectorized and aggregated formats. There is no differentiation between individual sectors in the GEOS-Chem simulation, so aggregated data was used. The most recent data was used (RETRO extends to the year 2000).

2.2   Conversion of RETRO species to GEOS-Chem tracers

The RETRO anthropogenic emissions inventory contains gridded data for 24 chemical species. For use in the GEOS-Chem model, these chemical species had to be converted to match 13 tracers in the ANTHSRCE diagnostic (Table 1).

Table 1: RETRO species to GEOS-Chem tracers

ANTHSRCE tracer	applicable RETRO species	comments
ALK4	Butanes	ALK4 is alkanes >= 4 carbon atoms
	Pentanes	
	Hexanes and Higher Alkanes	
ACET		Assume "Other Ketones" is all ketones other than acetone since a separate acetone category exists for biogenic data
MEK	Other Ketones	
ALD2	Other Alkanals	Assume all alkanals are acetaldehyde since no RCHO emissions are provided
RCHO		No anthropogenic emissions
PRPE	Propene	
C3H8	Propane	
CH2O	Methanal	
C2H6	Ethane	
BENZ	Benzene	
TOLU	Toluene	
XYLE	Xylene	
GLYX		No RETRO data
MGLY		No RETRO data
C2H4	Ethene	
C2H2	Ethyne	
HCOOH	Aggregated Acids	Assume HCOOH accounts for 25% of total acids based on Chebbi et al. (1996)
ACTA		

2.3   RETRO methodology

The RETRO anthropogenic emissions inventory was based largely off of previous work by the Netherlands Organisation for Applied Scientific Research (TNO) [1]. TNO developed a model for estimating emissions, called TNO Emissions Assessment Model (TEAM), which was based in turn off of an earlier project, Tropospheric Ozone and Precursors, Trends, Budgets, and Policy (TROTREP) [2].

The TROTREP team developed emissions and technology factors as well as rates of emissions for specific activities. TEAM was created to use these data to produce a gridded emissions inventory by compiling a database of technologies and their emission factors for each timestep and country [2]. The equation is as follows [1]:

$$E_{pollutant}(t) = \sum_{activities} \left(\sum_{technologies} \left(AR_{activity}(t) x P_{activity,technology}(t) x EF_{technology,pollutant} \right) \right)$$

In the equation above, AR is the Activity Rate of the process which produces emissions and can be found using economic data. P is the Penetration, the fraction of the activity performed using a specific technology. Penetration can be found by correlating activities with the technologies that they employ. EF is the Emission Factor, an attribute of the technology selected determining the linear relation between the activity rate and the resulting emission of a certain pollutant, using a specific technology. Because Penetration changes with time, Emission Factor can be independent. Emission Factor can be calculated using technological data for each region [2].

The RETRO team combined these factors with data from the International Energy Agency and an inventory for solvent use and biomass burning intended for input into modeling software [1]. These data were used with TEAM to produce a gridded global anthropogenic emissions dataset. The RETRO team then distributed national totals based on gridded population data from the Center for International Earth Science Information Network (CIESIN) to provide global gridded data [1]. NMVOCs were speciated based on country specific profiles developed in TROTREP. The resulting annual data was then divided into monthly data by LOTOS groups. To improve continuity, the data was smoothed before distribution.

3 Comparison of RETRO to existing GEOS-Chem inventories

3.1 Comparison to GEOS-Chem base inventory (GEIA)

To compare RETRO with the existing inventories, a GEOS-Chem simulation was run as follows:

- Version 8-02-01 dicarbonyls simulation
- Anthropogenic emissions and aerosols enabled
- Regional inventories disabled
- Timeframe Jan 01, 2000 to Jan 01, 2001
- ANTHSRCE diagnostic output included the 13 tracers provided by RETRO:
  - ALK4
  - ALD2
  - PRPE
  - C3H8
  - CH2O
  - C2H6
  - MEK
  - BENZ
  - TOLU
  - XYLE
  - C2H4
  - C2H2
  - HCOOH

The following figures compare output from two GEOS-Chem simulations: one with GEIA anthropogenic emissions and the other with RETRO anthropogenic emissions added in the update.
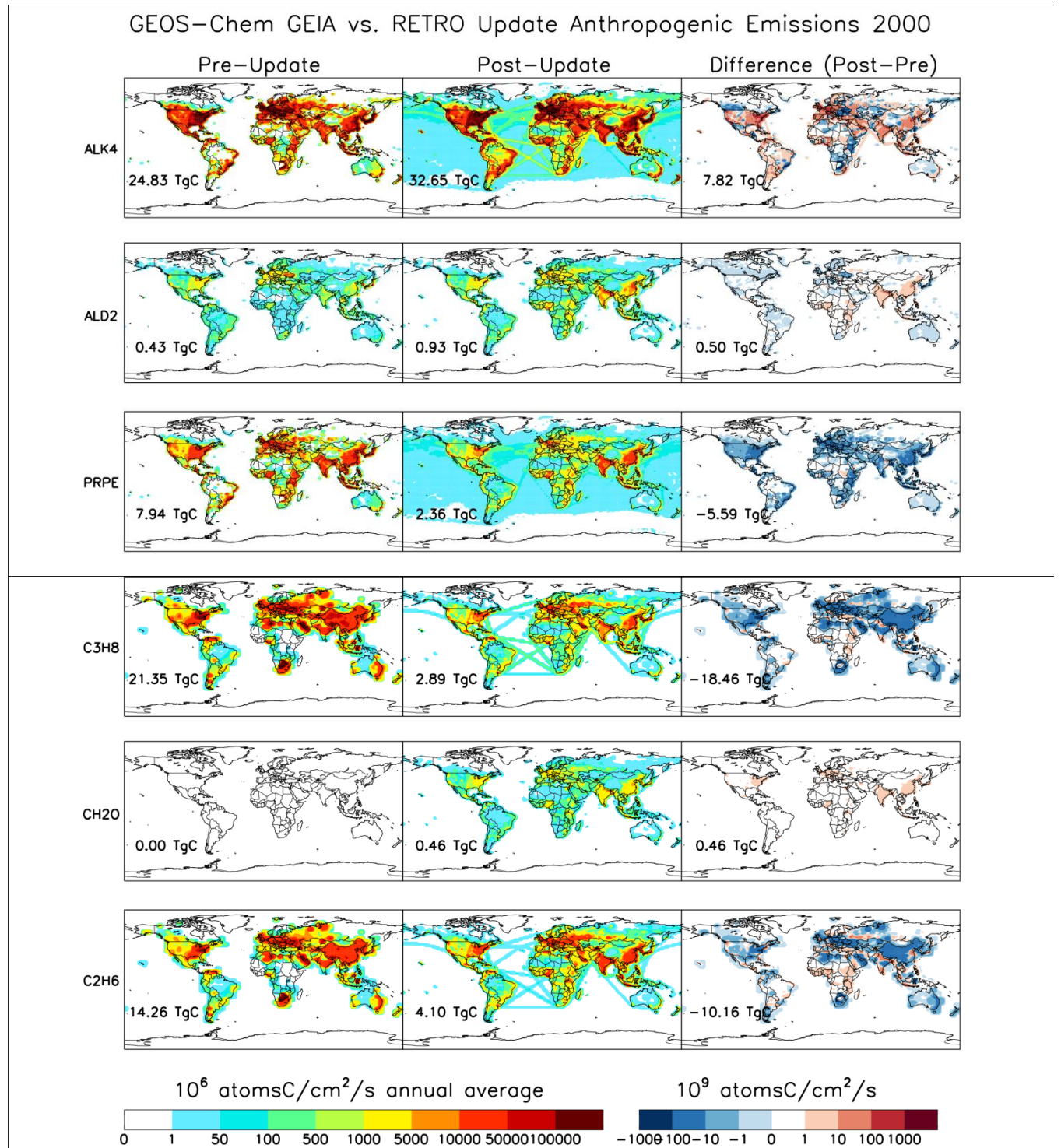
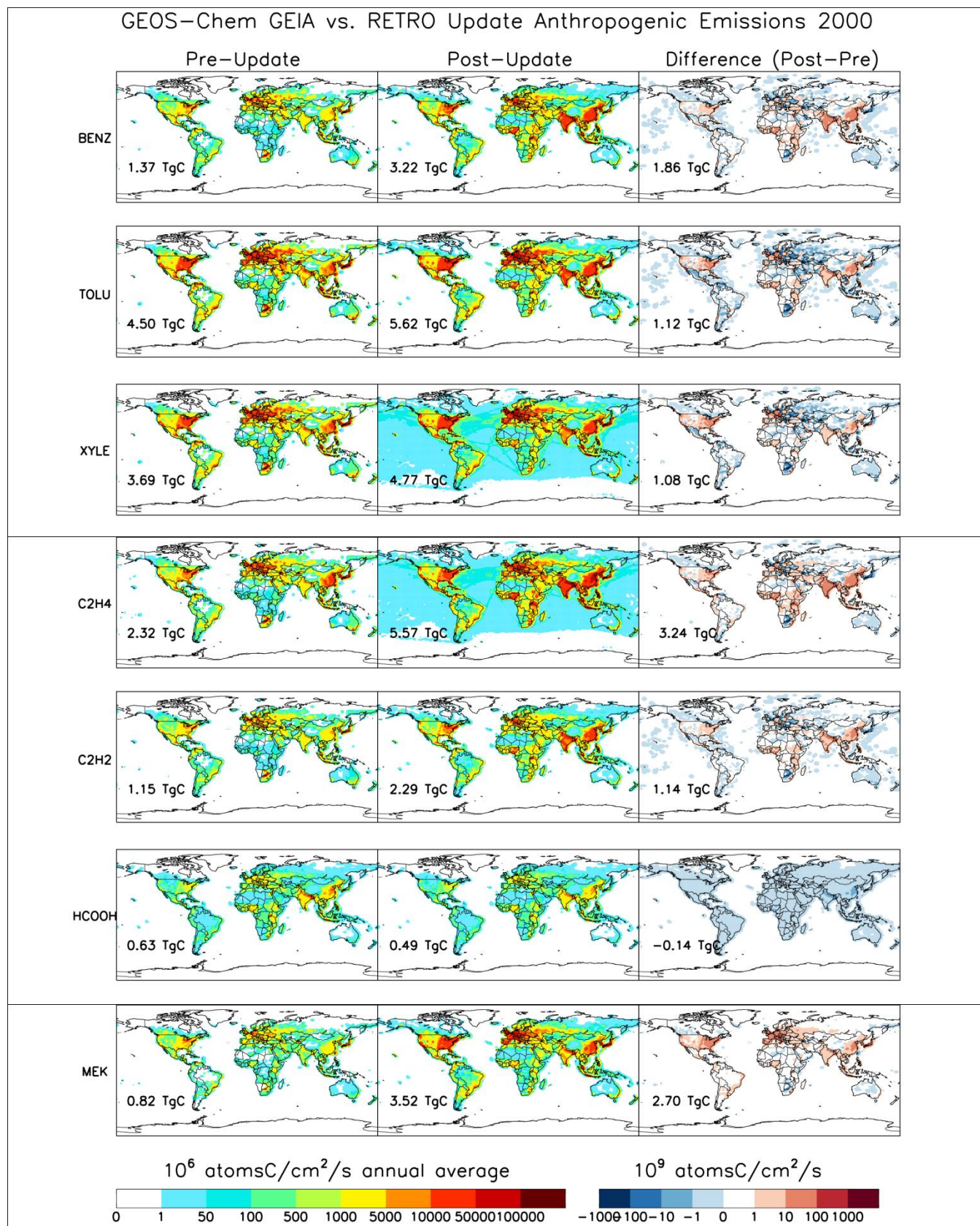**Figure 1:** GEIA vs. RETRO anthropogenic emissions simulation output for the year 2000

Figure 1 (ctd): GEIA vs. RETRO anthropogenic emissions simulation output for the year 2000

3.2 Comparison to GEOS-Chem EDGAR and regional inventories

GEOS-Chem allows for regional inventories to overwrite the base global inventory, GEIA, within defined geographic regions. These regional inventories often have finer spatial and temporal resolution than the base inventory. The RETRO inventory underwent comparison to these regional inventories as follows:

- Version 8-02-01 dicarbonyls simulation
- Anthropogenic emissions and aerosols enabled
- Optional/regional inventories enabled:
    - EMEP
    - BRAVO
    - STREETS
    - CAC
    - EPA/NEI99
    - EDGAR (optional global)
- Timeframe Jan 01, 2000 to Jan 01, 2001
- ANTHSRCE diagnostic output included the 13 tracers provided by RETRO:
    - ALK4
    - ALD2
    - PRPE
    - C3H8
    - CH2O
    - C2H6
    - MEK
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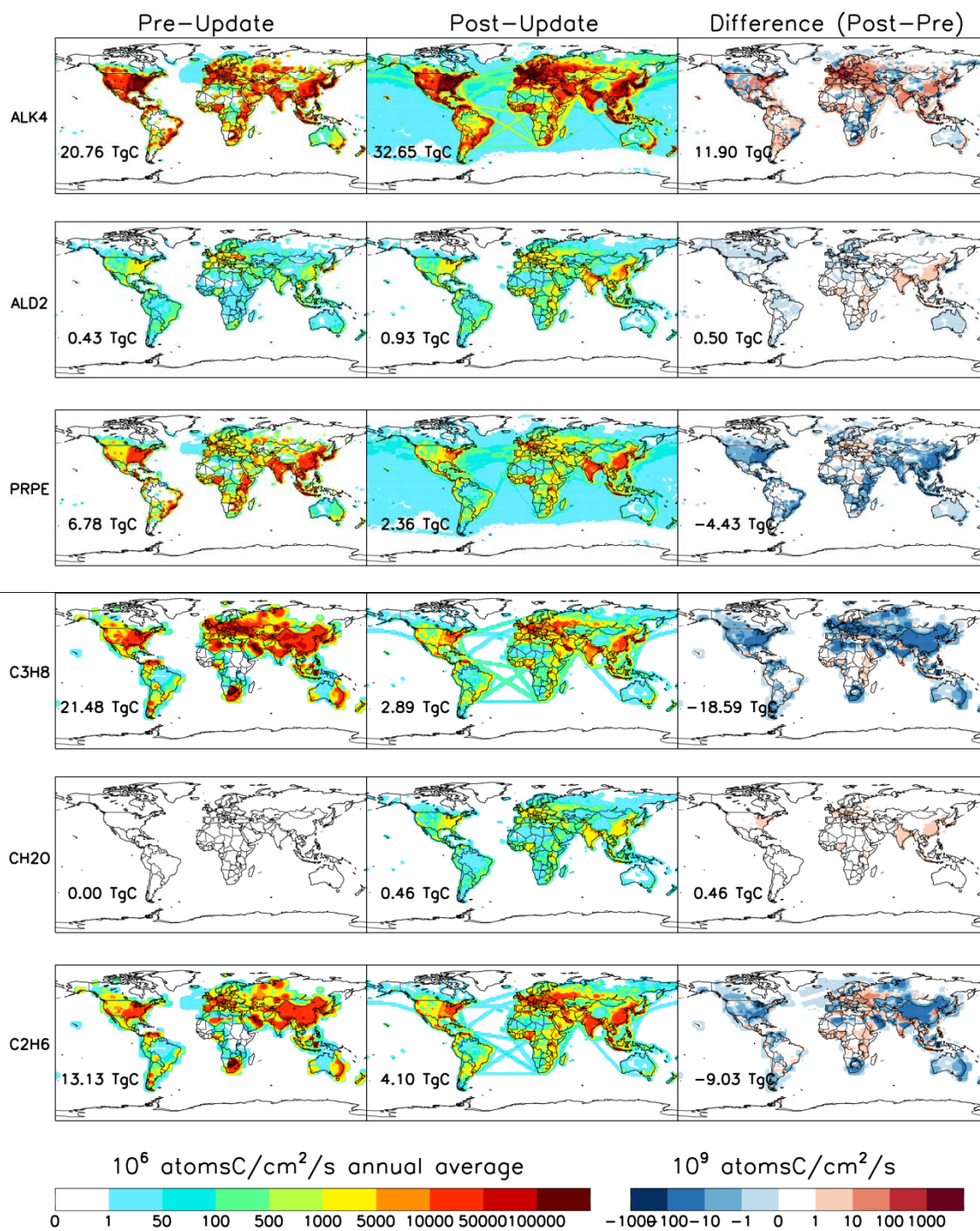
Figure 2: EDGAR and regional GEOS-Chem inventories vs. RETRO anthropogenic emissions simulation output for the year 2000
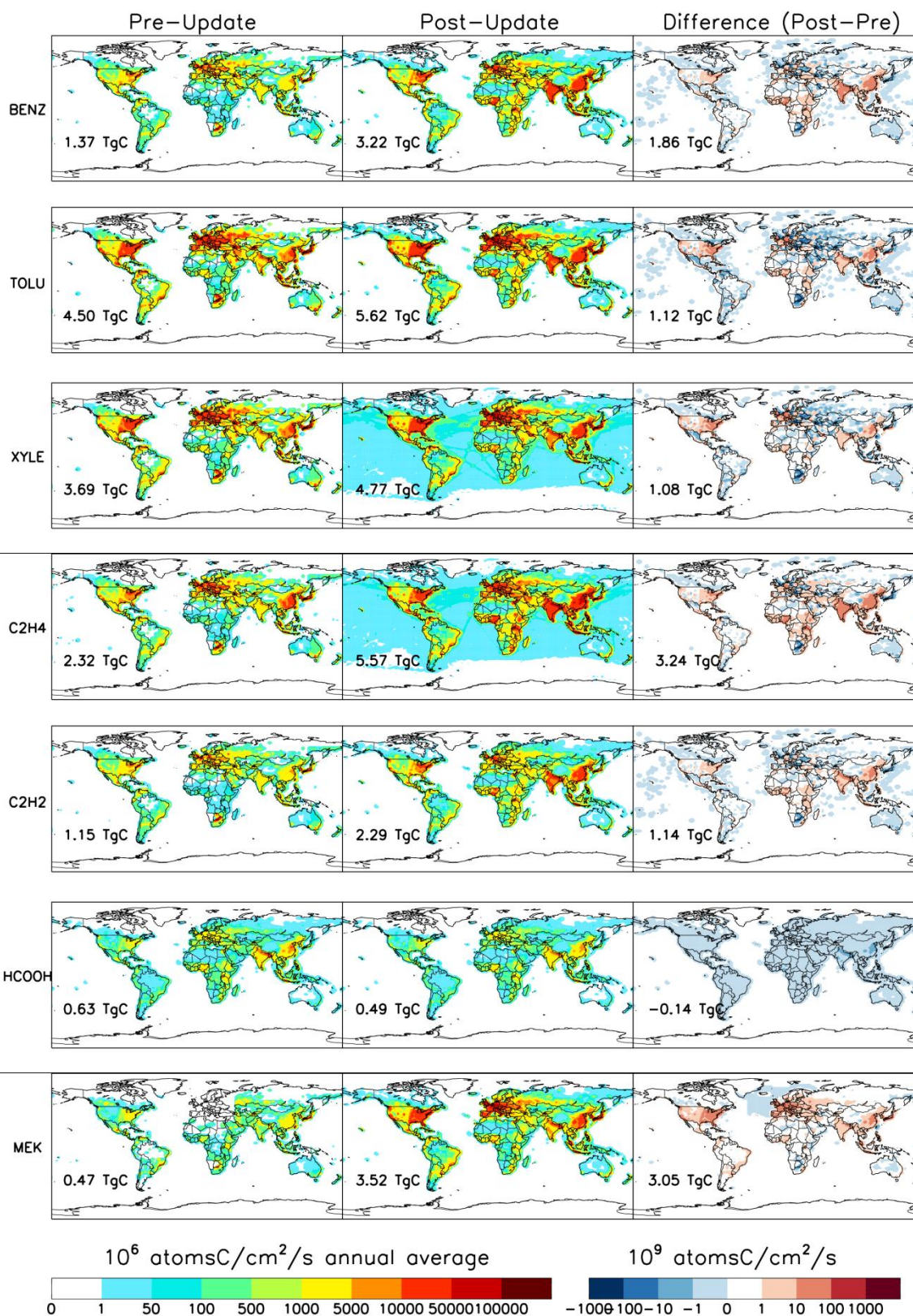
Figure 2 (ctd): EDGAR and regional GEOS-Chem inventories vs. RETRO anthropogenic emissions simulation output for the year 2000

3.3   Key points from comparison of RETRO to existing GEOS-Chem inventories

3.3.1   GEIA comparison

There was a large discrepancy for all tracers, but it was especially large for C3H8 and C2H6. GEIA flux was similar to RETRO in unpopulated areas, but was several orders of magnitude larger in densely populated areas. This suggests different methods of estimation over urban areas. We see this effect repeated for the PRPE tracer. ALK4, however, has the reverse effect; RETRO concentrations are higher than GEIA in populated areas and lower in unpopulated ones. No CH2O data were available in GEIA.

3.3.2   Regional comparison

The regional comparison revealed discrepancies similar to the GEIA comparison, although the regional inventories seemed to be in closer agreement with RETRO. C3H8 and C2H6 still had large differences, and ALK4 had a greater difference than with GEIA. No CH2O data were available in any of the regional inventories or EDGAR. RETRO's MEK emissions were significantly higher than the regional inventories over populated areas. It is also worth noting that MEK emissions from the EMEP inventory appeared erroneously low – on the order of 10^{-5} Tg annually. This was outside the scope of the update and therefore was not investigated.

4   Modification of GEOS-Chem

GEOS-Chem version 8-02-01 was modified to read in RETRO anthropogenic emissions as a base for global NMVOC emissions. The use of the RETRO inventory can be toggled with a switch in the emissions menu of /run_directory/input.geos. The RETRO emissions are overwritten by any regional inventories that are enabled from within input.geos. The following programs were modified to allow RETRO data to be read in:

Table 2: List of modified programs

directory	program(s)
/code_directory/	anthroems.f
	cleanup.f
	emfossil.f
	emissions_mod.f
	epa_nei_mod.f
	input_mod.f
	logical_mod.f
	Makefile
/run_directory/	input.geos

In addition to the modification of the programs above, the program retro_mod.f was created, using epa_nei_mod.f as a framework. The EPA/NEI routines were used because of the shared monthly temporal resolution and the number of common tracers between the EPA/NEI inventory and RETRO.

During the course of updating the model to read in RETRO emissions, it was also discovered that epa_nei_mod.f was written to read in CH2O data that did not exist, causing the simulation to show zero CH2O emissions over the US. This was corrected with small modifications to epa_nei_mod.f and emfossil.f which prevent emissions being set if no data is found.

5   References

1. Bolshcer, M, et al., *RETRO Deliverable D1-6*, RETRO Documentation, 2007.
2. Pulles, T, et al., *Assessment of Global Emissions from Fuel Combustion in the Final Decades of the 20th Century*, TNO report A-R0132/B, 2007.